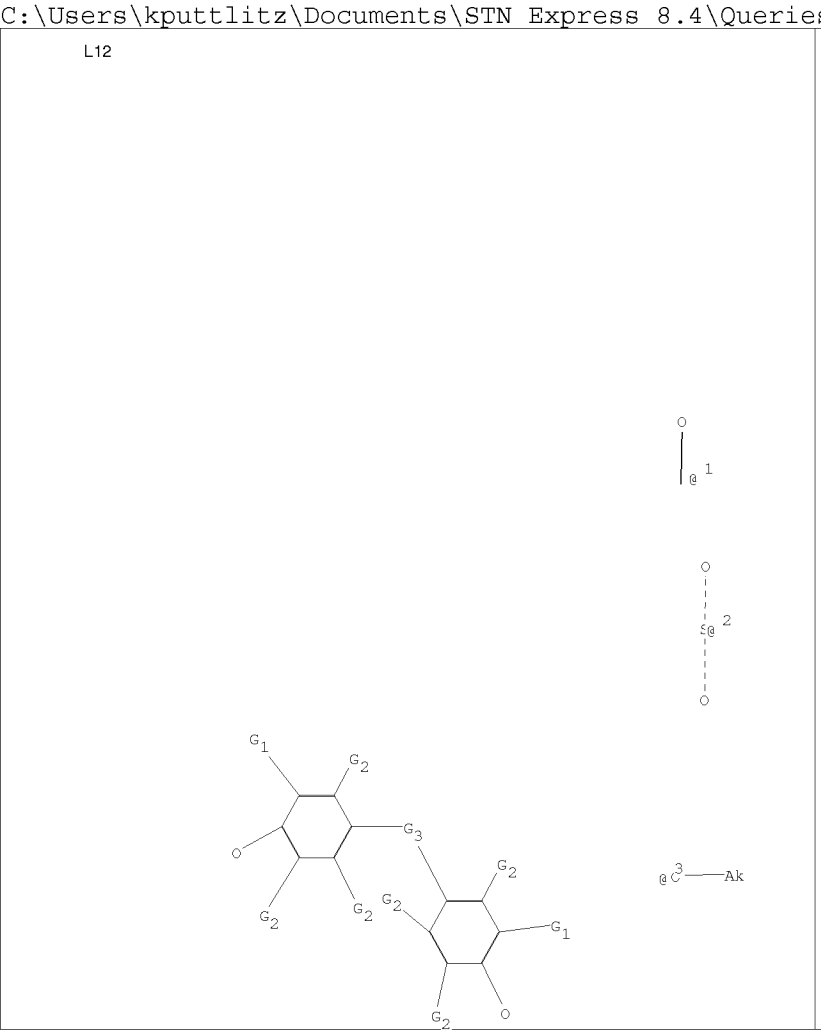
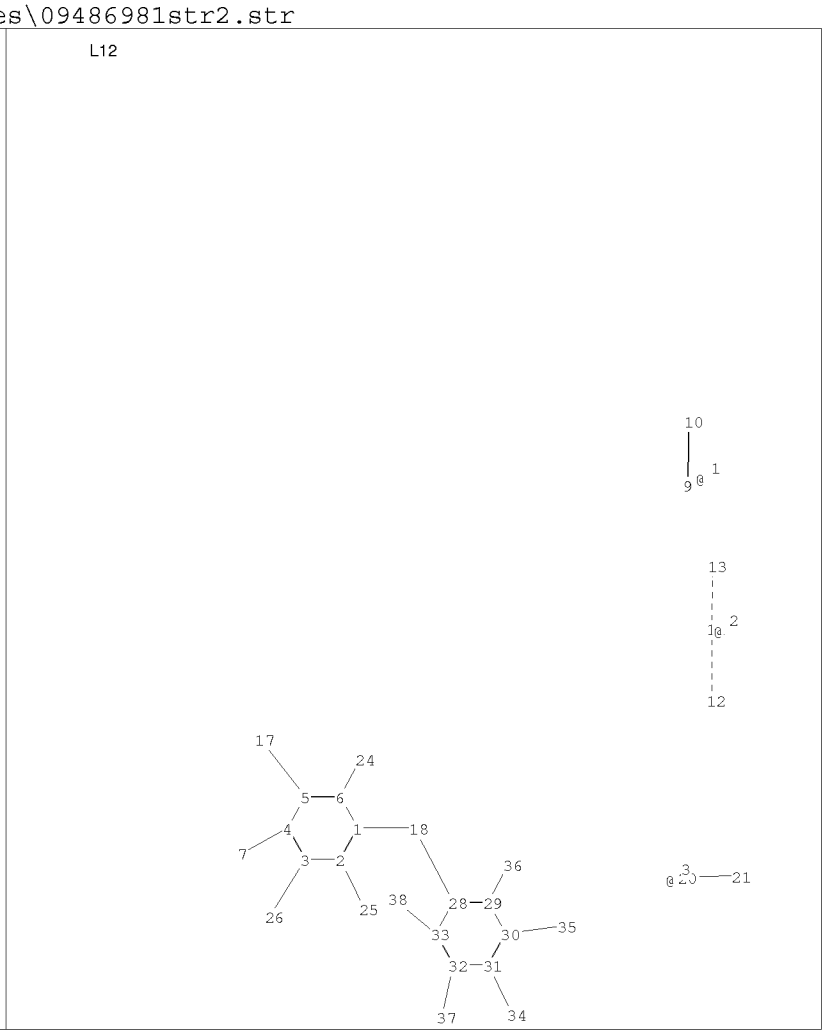
C:\Users\kputtlitz\Documents\STN Express 8.4\Queries\09486981str2.str





chain nodes :
7 9 10 11 12 13 17 18 20 21 24 25 26 34 35 36 37 38
ring nodes :
1 2 3 4 5 6 28 29 30 31 32 33
chain bonds :
1-18 2-25 3-26 4-7 5-17 6-24 9-10 11-12 11-13 18-28 20-21 29-36 30-35 31-34 32-37
33-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 28-29 28-33 29-30 30-31 31-32 32-33
exact/norm bonds :
1-18 2-25 3-26 4-7 5-17 6-24 9-10 11-12 11-13 18-28 20-21 29-36 30-35 31-34 32-37
33-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 28-29 28-33 29-30 30-31 31-32 32-33

G1:[@1],[@2]

G2:H,X,Ak,[@1],[@2],[@3]

G3:C,O,S

Hydrogen count :
7:>= minimum 1 34:>= minimum 1
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS